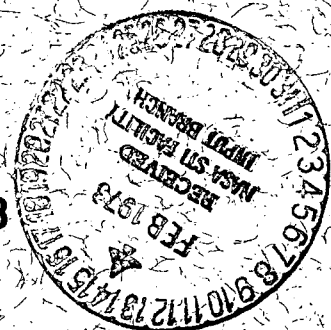NASA TM X- *66171*

REPORT OF TASK GROUP II TO COESA

PROPOSED REVISION TO THE U. S. STANDARD
ATMOSPHERE 86 TO 200 KM

JANUARY 1973

GSFC ——— **GODDARD SPACE FLIGHT CENTER** ———
GREENBELT, MARYLAND

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ATMOSPHERE 86 TO 200 KM

Prepared by Task Group II

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I. INTRODUCTION

A meeting of the committee for the Extension to the U.S. Standard
Atmosphere (COESA), was held in Boston on September 13, 14, and 15, 1971.
At this meeting it was agreed to review the current state of knowledge
of the earth's atmosphere with the objective of possibly revising the
"U. S. Standard Atmosphere, 1962" above the altitude of 50-60 km, and
of extending the upper limit of the tabulations of a revised standard
to 1000 km.

Various schemes have been used to divide the vertical extent of
the atmosphere into a number of regions. One of these is based upon
the major features of the temperature-height profile. Another is based
upon major features in height distribution of the constituent gases of
the atmosphere. In order to facilitate the review of data and the re-
vision of the "U.S. Standard Atmosphere, 1962" COESA has chosen to
divide the atmosphere in accordance with a two-fold criterion:

(1) the principal techniques used for measuring the thermodynamic
properties of the atmosphere (temperature, density and pressure) and

(2) the amount of observational data available for constructing
and testing any proposed model. Applying this criterion of measuring
technique and quantity of data within the height region of interest,
50 to 1000 km, COESA has divided the atmosphere into three overlapping
regions, and has assigned a particular task group to concentrate on
each of these three regions:

Task Group I,   50 to 100 km

Task Group II,   80 to 200 km

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Task Group III, 140 to 1000 km

The height region for Task Group I, 50 to 100 km, is a region in which atmospheric measurements of temperature, density and pressure are made almost exclusively with rocket-borne instruments; these have served to develop an extensive set of thermodynamic data. The height region for Task Group III is one in which the thermodynamic properties are determined almost exclusively from satellite related observations: A vast amount of data, particularly mass-density data has been accumulated for this height region, 140 to 1000 km.

The height region for Task Group II, primarily the 40 kilometers between 100 and 140 km, plus an overlap into the regions of the other two task groups is a region for which niether the rocket-related observations nor the satellite-related observations provide much information. No unique vehicle or observational technique has to date been developed for efficient observation of this height region, and only a limited amount of thermodynamic data for this region were available for consideration by Task Group II; consequently, the job of Task Group II became primarily one of fitting an analytical function to bridge the gap between models which were appropriate to the other two regions.

Task Group II met on four different occasions

February 22, 1972	GSFC	Greenbelt, Maryland
April 19, 1972	Sheraton Park Hotel, Washington, D.C.	
November 3, 1972	GSFC	Greenbelt, Maryland
December 8, 1972	AFCRL	Bedford, Massachusetts

with Champion, Reber and Minzner in attendance at each of these meetings

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and with other members absent from one or more meetings. Only two basic proposals were submitted to the committee, one by G. R. Swenson, and one by C. A. Reber. The first two meetings were devoted to the discussion of these proposals, with successive revisions between meetings. By the third meeting, some of the differences between these two proposals had been resolved and Swenson withdrew his proposal in favor of the successively revised Reber model. At this meeting empirical number-density concentrations of various atmospheric species were agreed upon by the committee for the 150-km height level. Some revisions to eddy diffusion coefficients were also suggested. To achieve the recommended N_2 densities as well as to incorporate some recommended revisions in Reber's temperature-height profile, in the 100-115 km region, it became necessary to lower the temperature in the 86 to 90 km region. This was accomplished by a revision of the model of Task Group I through coordination with that group.

At the December meeting the nth version of the Reber model was reviewed, and further modifications were suggested. One member who had made no overall proposal still had misgivings, but the committee agreed to adopt, for submission to COESA, the Reber model of that date with yet a few modifications.

Various members of the committee agreed to participate in the preparation of the report as follows:

Principal Discussion of the Model   -- Reber

Composition Measurements   -- Nier and Moe

Eddy Diffusion Considerations   -- Zimmerman

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II. LOWER BOUNDARY CONDITION

Because of the necessity for continuity with the "U.S. Standard Atmosphere, 1962" at a height of 50 kilometers, it was necessary for the several task groups to generate their respective models sequentially. Task Group II would therefore use the temperature and density of the model of Task Group I, at some point in the overlap region between 80 and 100 km, as the lower boundary values for its model.

The purpose of the regions of overlap for the three task groups was to allow needed flexibility in the generation and matching of the successive models. For example, the temperatures in the recommended isothermal region between 85 and 90 geopotential kilometers as orig- inally submitted by Task Group I were sufficiently high so that no rea- sonable temperature-height profile above 100 km would yield acceptable densities at 150 km. In the ensuing coordination between Task Group II and Task Group I it was finally agreed that the temperature gradient of -1.8 Kelvin degrees per geopotential kilometer (K/km') between 71 and 85 km' would be changed to -2.0 K/km', thereby producing a reduction of 2.8 K (from 189.45 K to 186.65 K) at 85 geopotential kilometers (km'), and simultaneously allowing for an acceptable value of mass density at 150 km geometric kilometers (km) with a reasonable temperature profile between 85 km' and 150 km. (The above revision was preferred by Task Group I over a proposed extension of the -1.8 K/km' gradient from 85 km'

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to 86.5 km' whereby the temperature of the isothermal layer would have been reduced from 189.45 to 186.75 K, while the base of this layer would have been raised 1.5 km'.

The transition region between the temperature profile of the model of Task Group I and that of Task Group II also serves as a region of transition between two different scales of temperature, (i.e. molecular scale temperature T_M, and kinetic temperature T) as well as between two different scales of height measurement (i.e., standard geopotential kilometers km', and geometric kilometers km). In the "U.S. Standard Atmosphere, 1962", the model was divided at 90 geometric kilometers with that part from 0 to 90 km defined in terms of T_M and H, and the part above 90 km defined in terms of T and Z. A similar policy is being followed in the proposed revisions to the 1962 Standard. It is the recommendation of Task Group II, however, that the height at which this transition occurs be set at 86 geometric kilometers, or 84.8520 km' where the molecular scale temperature according to the revised model of Task Group I is 186.9460 K. It is desirable that the transition occur at an integer value of geometric height measure for ease in integration at higher altitudes in intervals of one geometric kilometer.

Because the model being proposed by Task Group II implies the existance of some atomic oxygen at 86 km, the mean molecular weight M applying to that height has been taken to be 28.940. At this height the ratio M/M_o, therefore, has the value

$$(28.940/28.9644) = .9991645$$

and the kinetic temperature has the value of 186.789805 which when

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rounded to 5 significant figures is 186.79K. Using a Task Group I value

of 6.421062 X 10^{-5} kg/m^3 for the density at 71 km where the value of

T_M is 214.65 K, and assuming a constant gradient of -2K/km from

71 km to 84.8520 km or 86.000 km where the value of T_M must therefore

be 186.9460 K, the value of density has been computed to be 6.957839 x

10^{-6} kg/m^3. The values representing the boundary conditions for the

lower end of that portion of the Proposed Standard Atmosphere above

86 km as recommended by Task Group II, are therefore as follows:

H = 84.8520 km

Z = 86 km

M/M_o = .9991645

T_M = 186.9460 K

T = 186.7898 K

A brief discussion of history of the development and use of

molecular scale temperature and geopotential is given in the Appendix.

III. PHILOSOPHY AND CONSTRAINTS OF THE MODEL

In addition to the basic guidelines already mentioned, it was

felt that the form of the mathematical expressions defining the temp-

erature and number-density profiles as a function of altitude should

make the model useful as a theoretical tool throughout the altitude

range. A number of implications follow from this philosophy:

a. The temperature should be expressable as a smooth mathematical

function of geometric altitude, with a smooth second derivative. In

particular, it was felt desirable to use the exponential (Bates, 1959)

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profile in the middle and upper thermosphere as this form is well known, widely used, and permits the utilization of the Walker (1965; Bates, 1959) technique for analytically representing upper atmosphere number densities.

b. The functions representing the temperature profile should be readily adjustable to allow approximation of varied data sets.

c. The functions relating number densities to altitude should be physically meaningful and expressable analytically.

The temperatures and gas-specie number densities of the model have to be consistent with inputs from a variety of sources:

a. At the lower altitude boundary the temperature and number densities must match with the model recommendations of Task Group I, a match which is somewhat complicated by the fact that the model of TGI is defined in terms of geopotential altitude and molecular scale temperature, while TG II uses geometric altitude and kinetic temperature (see Section II).

b. In the region between the lower boundary and about 130 km, the temperature and mass density profiles should match the data available, which come largely from rocket-borne pitot measurements, falling-sphere measurements and Thomson incoherent scatter measurements. However, the average value of the N_2 density above 150 km is fairly well established, and this has a large influence on the choice of temperature profiles in the region below this altitude. See the discussion in IV.C.1.

c. At 150 km the composition should match the TG II recommendations shown in Table I and discussed in Section V.

d. The largest body of data available on the neutral composition of the thermosphere (as opposed to the larger data set available on total density) was that obtained from the quadrupole mass spectrometer on the OGO-6 satellite (e.g. Hedin, et al., 1972). Since these data are referenced primarily to an altitude of 450 km it was decided to extend the calculations for the Task Group II model to at least that altitude to allow inclusion of this large and unique data set. (Table I)

e. The decision had been made by the COESA at the September 1971 meeting that the average conditions to be modeled could be well approximated by using an exospheric temperature of 1000°K.

f. At altitudes above about 150 km, the total density and its scale height should be consistent with the large body of data determined from satellite drag.

It has been borne in mind throughout that many of the parameters and profiles used and calculated are dynamic by nature and any steady-state description is only an approximation to the true state-of-affairs. Examples are the temperature profile which generally exhibits wave-like structure, the atomic oxygen profile which calculations show to be extremely time dependent with a significant diurnal component, and the helium profile with an annual component. For the purposes of this model, choices were made for the best average value or profile to be used or matched.

IV. MODEL

A. Temperature

The temperature profile is described in four altitude ranges:

1. z_o (86 km) to z_1 (91 km): isothermal at $186.79°K$.

2. z_1 (91 km) to z_2 (110 km): A portion of an ellipse is used here, assuring a smoothly monotonically increasing temperature with altitude, with sufficient generality to match the temperature and its gradient at the end points of the region of definition.

$$T(z) = T_c + b^2 \left(1 - \frac{(z-z_1)^2}{a^2}\right)^{1/2} \tag{1}$$

where

$$T_c = \frac{YT_2 - T_2^2 + T_1^2}{Y + 2T_1 - 2T_2} \; ,$$

$$Y = \frac{dt}{dz}\bigg|_{110} (z_2 - z_1) \; ,$$

$$a = \frac{b \, (z_2 - z_1)}{(b^2 - (T_2 - T_c)^2)^{1/2}} \; ,$$

$$b = (T_1 - T_c).$$

3. z_2 (110 km) to z_3 (125 km):

$$\frac{dT(z)}{dz} = 12°/km \quad ,$$

$$T_2 = 240°K, \text{ and}$$

$$T_3 = 420°K.$$

4. z_3 (125 km) to 500 km:

$$T(z) = T_\infty - (T_\infty - T_3) \exp(-\sigma \, \xi), \qquad (2)$$

where T_∞ = exospheric temperature

$$\sigma = \frac{1}{T_\infty - T_3} \left. \frac{dT}{dz} \right|_{z_3} = 0.02069 \text{ km}^{-1},$$

$$\xi(z) = \frac{(z - z_3)(R + z_3)}{R + z}, \text{ and}$$

$$R = \text{earth radius} = 6356.77 \text{ km}.$$

B. Densities

The steady-state vertical distribution of a minor gas specie of number density n_i and mass m_i is governed by the vertical component of the momentum equation for that gas (e.g. Colegrove, et al., 1965):

$$n_i v_i + D_i \left(\frac{dn_i}{dz} + \frac{(1 + \alpha_i)}{T} \frac{n \, dT}{dz} + \frac{n_i}{H_i} \right)$$

$$+ K \left(\frac{dn_i}{dz} + \frac{1}{T} \frac{dT}{dz} + \frac{n_i}{H} \right) = 0; \qquad (3)$$

where v_i = the flow velocity of ith specie,

D_i = local molecular diffusion coefficient for i^{th} specie diffusing through the major, background gas,

α_i = thermal diffusion factor for i

(= -0.4 for He; = 0 for all others),

$H_i = \frac{kT}{m_i g}$ = local scale height for i,

k = Boltzmann constant,

g = local acceleration of gravity,

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K = eddy diffusion coefficient,

$H = \dfrac{kT}{Mg}$ = local scale height of the atmosphere, and

M = local mean molecular mass of the atmosphere.

1. Molecular nitrogen

Equation 3 is used to calculate the distribution of each gas except molecular nitrogen; since N_2 is the major gas in the lower part of the thermosphere a different scheme is used to describe its distribution. From the lower boundary altitude of 86 km up to about 100 km the atmosphere is well mixed, as the eddy processes dominate the molecular diffusion, while above about 100 km molecular diffusion dominates. Also, because the molecular mass of N_2 (28.0134 amu) is quite close to the mean mass of the atmosphere before dissociation and diffusion become important (28.9644), the transition from mixing to a diffusive distribution has little effect on the vertical distribution of molecular nitrogen. This allows the use of a simplified version of Equation 3 for N_2, with the flow and the eddy terms set equal to 0:

$$\frac{dn\,(N_2)}{dz} + \frac{1}{T}\frac{dT}{dz} + \frac{n(N_2)}{H_{N_2}} = 0.$$

Thus, the distribution of molecular nitrogen is affected only by the temperature profile. To account for the slight change from mixing to diffusion, the mean mass is used in the calculation from 86 km to 100 km, and the N_2 mass is used above 100 km.

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2. Atomic and Molecular Oxygen, Helium and Argon

Ideally, Equation 3 is solved in conjunction with the equation of continuity (Colegrove, et al., 1965; Keneshea and Zimmerman, 1970),

$$\frac{d}{dz} (n_i v_i) = S (z)$$

where S denotes production and loss terms. However, for the purpose of the single-profile, steady-state model being generated here, it was felt that a sophisticated and detailed calculation of this nature was not appropriate. Instead the flux terms, $n_i v_i$, is artificially adjusted to include the effect of photo chemical production and loss on the vertical distributions of atomic and molecular oxygen. For helium and argon the flux term represents only the vertical flow.

Equation 3 is integrated directly to obtain

$$n_i(z) = \frac{n_i(z_0) T(z_0)}{T(z)} \exp \left[- \int_{z_0}^{z} (f(z) + \frac{v_i}{D_i + K}) \, dz \right], \qquad (4)$$

where

$$f(z) = \frac{D_i}{H_i (D_i + K)} + \frac{D_i(1+\alpha)+K}{T(D_i+K)} \frac{dT}{dz} + \frac{K}{H(D_i + K)} .$$

The eddy diffusion coefficient profile used in the calculation is of the form (Appendix II).

$$K(z) = 3.0 \times 10^7 \exp \left(\frac{-2.303 \ (z-88)}{2 \ 5}\right)^2 , \ z \leq 88 \text{ km}$$

$$= 3.0 \times 10^7 \exp \left(\frac{-2.303 \ (z-88)}{8}\right)^2 , \ z \geq 88 \text{ km}.$$

The molecular diffusion coefficients represent diffusion through molecular nitrogen, and have the general form

$$D_i(z) = \frac{\alpha_i}{N(z)} \left(\frac{T(z)}{273.16} \right)^{\beta_i} \frac{cm^2}{sec} \quad ,$$

where $N(z)$ is the total number density. The coefficients α and β are

listed in Table II. The calculation of the total number density used

for $D_i(z)$ is done sequentially, with N_2 providing the $N(z)$ for the

calculation of the atomic and molecular oxygen diffusion coefficients,

and $n(N_2) + n(0) + n(0_2)$ providing $N(z)$ for the argon and helium coefficients.

The flux term, $\frac{v_i}{D_i + K}$, in Equation 4 is represented by the integrable

expression

$$\frac{v_i}{D_i + K} = A_1(z-a_1)^2 \exp(-b_1(z-a_1)^3) + A_2(a_2-z)^2 \exp(-b_2(a_2-z)^3).$$

The constants A_1, A_2, a_1, a_2, b_1, and b_2 are determined such that appro-

priate densities are determined at 450 km for 0 and He, and at 150 km

for 0, 0_2, He and Ar. The constant $A_2 = 0$ for all species except

atomic oxygen; the extra term for 0 is needed to generate a maximum in

the density profile(chosen to be at 97 km), reflecting the increased

loss by recombination at lower altitudes. The flux terms for 0 and 0_2

are based on, and lead (qualitatively) to the same results as those

derived from the much more detailed calculations by Colegrove, et al. (1965)

and Keneshea and Zimmerman (1970). Table II lists these coefficients.

C. Discussion

1. N_2 density and the temperature profile

As noted in paragraph B.1, the N_2 density at any altitude is

sensitive primarily to the temperature profile at lower altitudes.

This fact has serious implications when there are a number of data sets

to be matched, as in the case here, where the lower boundary conditions are given (at 86 km), a density for N_2 at 150 km is given, and there are some temperature data available in the region between these two altitudes.

The temperature data consist mainly of recent pitot-tube measurements (J. Theon and J. Horvath, private communication) and incoherent scatter measurement (e.g. R. Wand, private communication). These two data sets are quite consistent in one particular feature: the temperature profile between about 105 km and 125 km appears to have a constant gradient of approximately 18°/km. The proposed model does, in fact, exhibit a constant gradient in this region, but it is 12°/km, only 2/3 of the measured value. Attempts to incorporate higher gradients lead to unacceptably high values for N_2 densities above 150 km, and herein lies the dilemma.

The lower boundary parameters and the N_2 density at 150 km reflect the results of many measurements in which there is a high degree of confidence so it is not likely that these data are in error. It is not clear whether the recent measurements of the temperature profile over estimate the gradient, or whether the three inputs are inconsistent in that they are not true averages over the same sets of conditions.

2. Dynamic characteristics

As noted earlier, most of the properties being modeled are time-dependent by nature, and any steady-state description has to be used advisedly. Examples are the diurnal photo-chemical variations in atomic and molecular oxygen densities and the longer term, dynamically induced variations in helium and argon densities. The proposed model

TABLE I

MOLECULAR DIFFUSION AND FLUX COEFFICIENTS

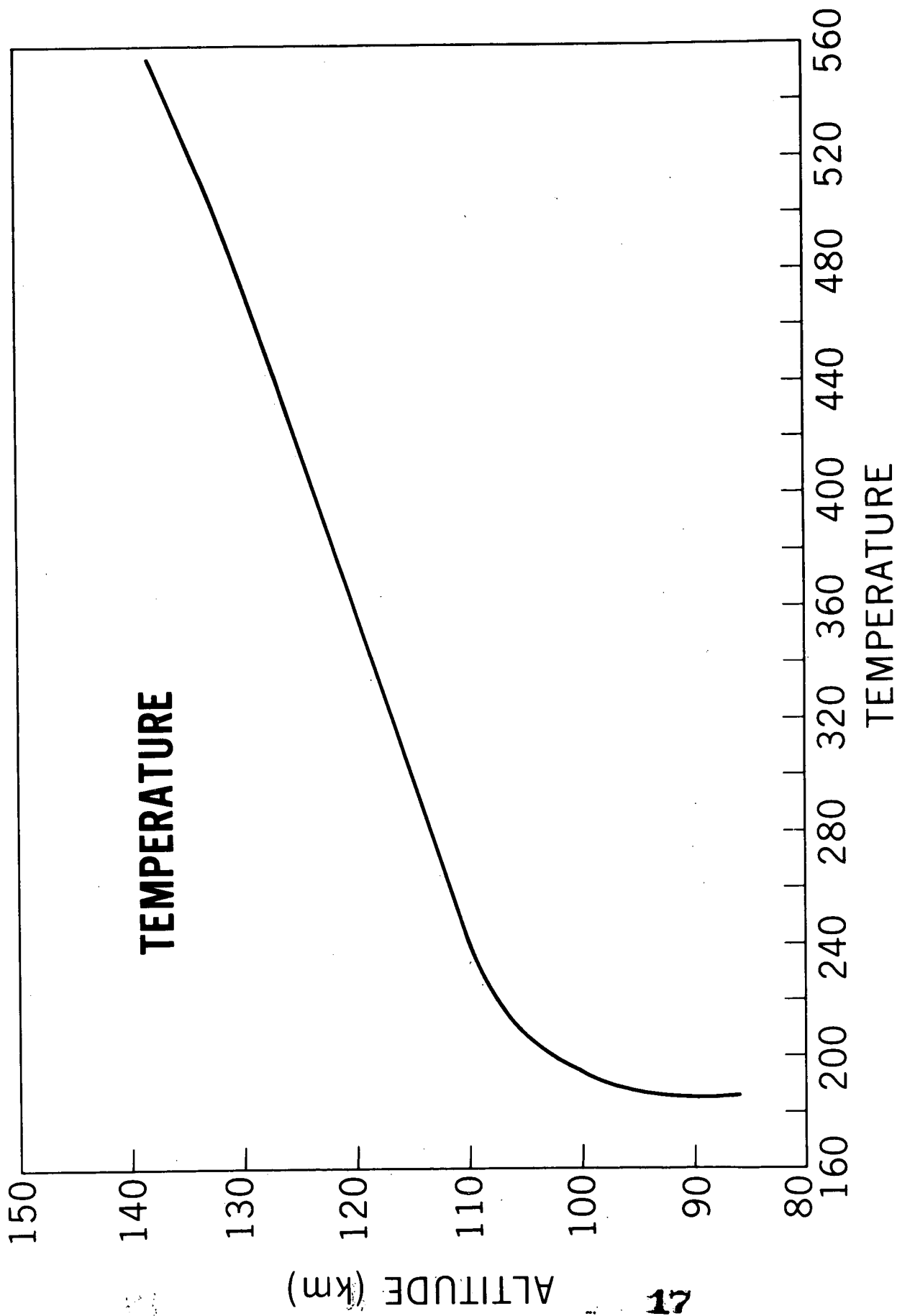|	Atomic Oxygen	Molecular Oxygen	Argon	Helium
α^*	6.9862×10^{18}	4.8635×10^{18}	4.4873×10^{18}	1.701×10^{19}
β^*	0.75	0.75	0.87	0.691
A_1	5.0565×10^{-3}	1.1549×10^{-4} **	9.5393×10^{-6} **	6.8068×10^{-4}
A_2	-4.6299×10^{-3}	0	0	0
a_1	69.02	105	105	87
a_2	10.0			
b_1	5.0088×10^{-4}	8.3333×10^{-5}	8.3333	6.6667×10^{-4}
b_2	1.4788×10^{-4}	----	----	----

*(Referenced in Colegrove, F. D., F. S. Johnson, and W. B. Hanson, "Atmospheric Composition in the lower thermosphere", J. Geophys. Res., 71, 2227, 1966.)
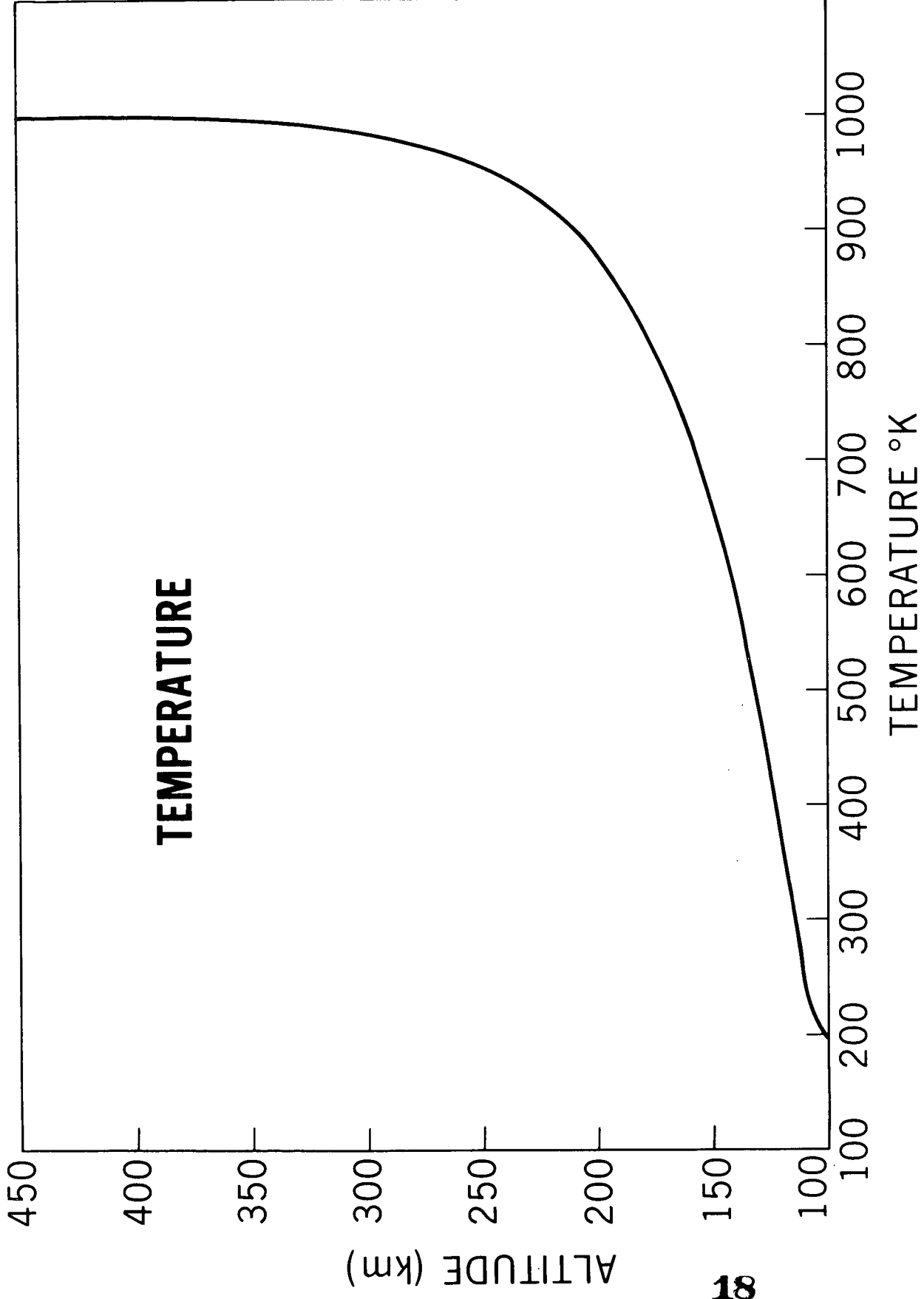
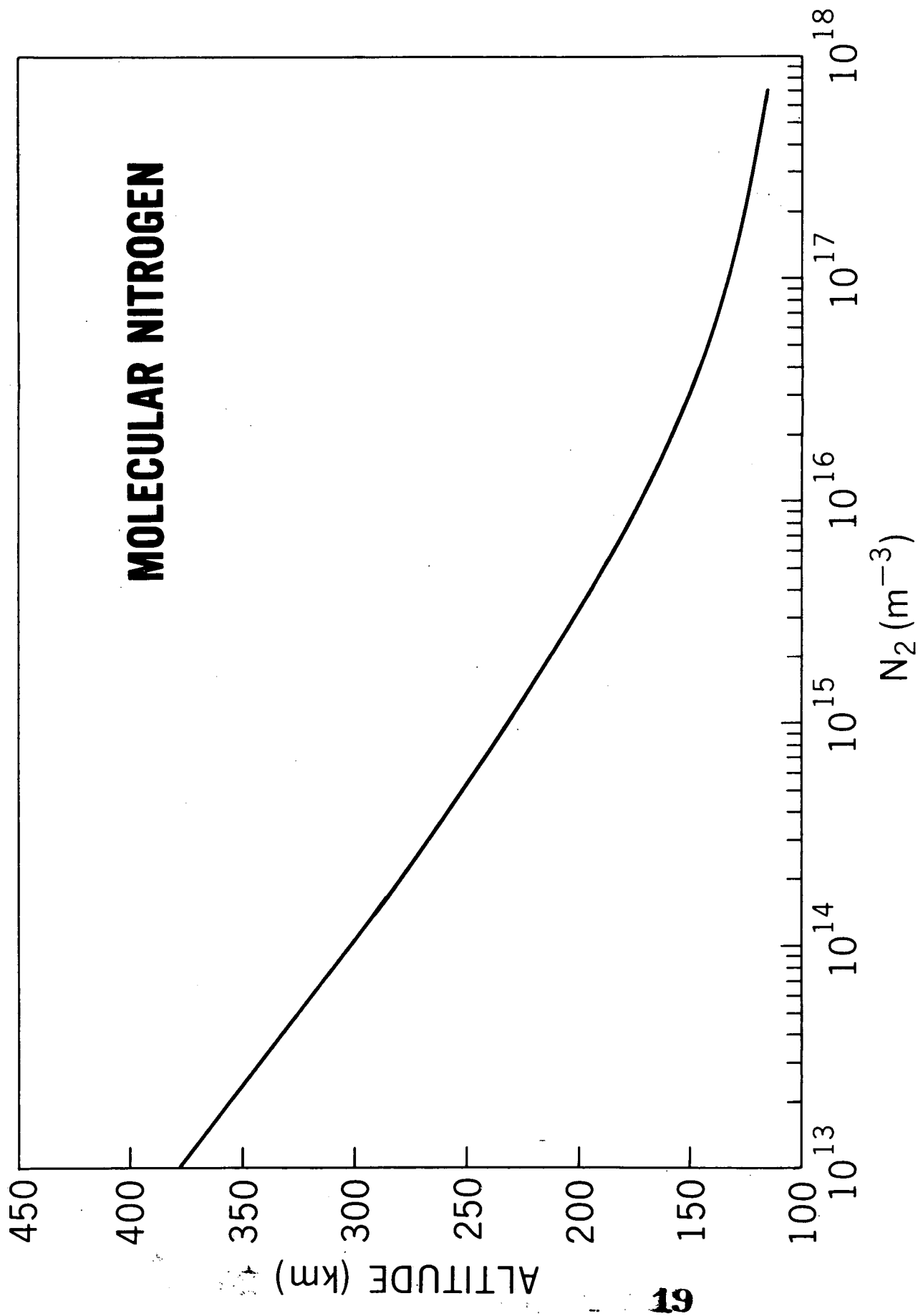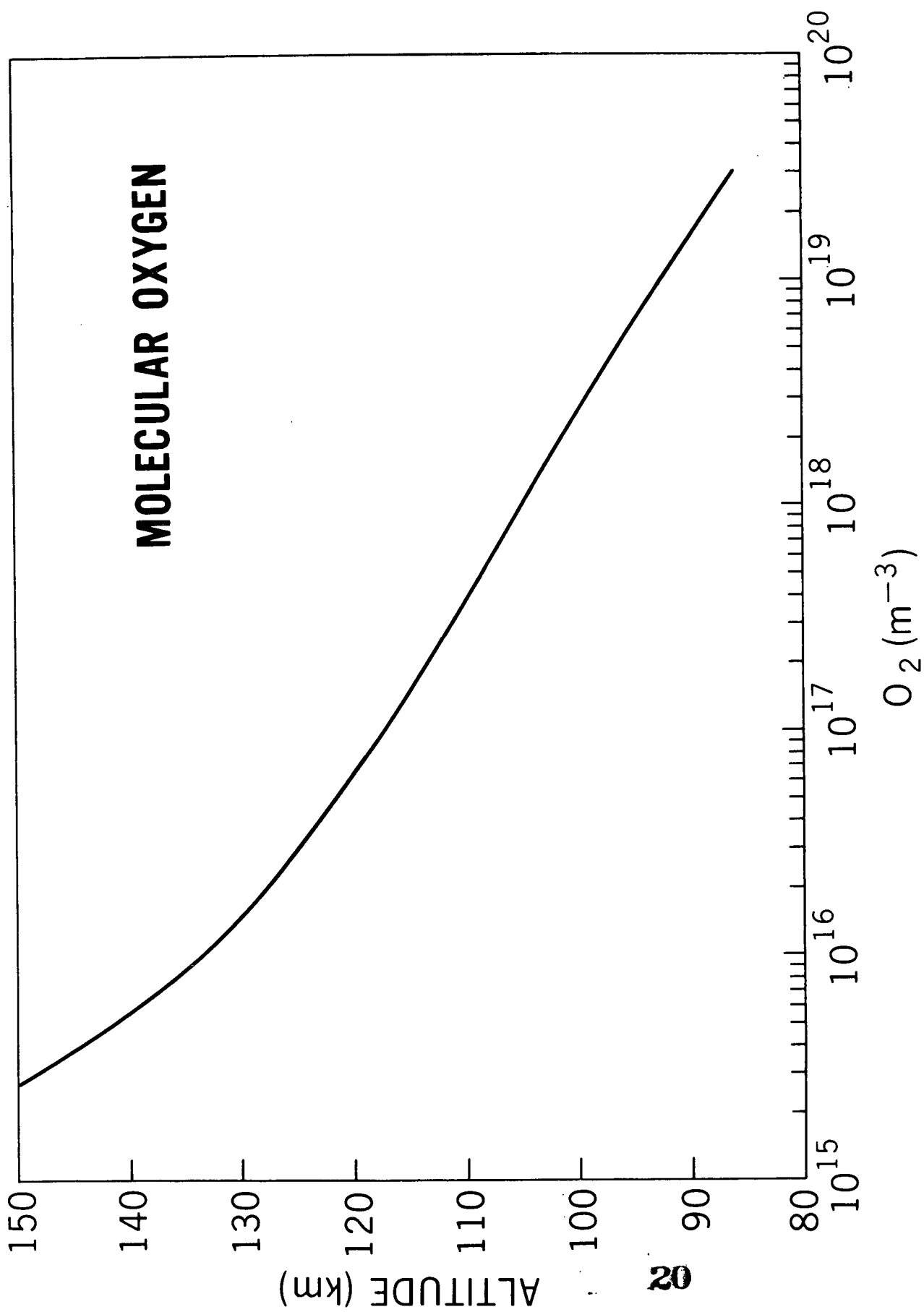**only defined for $z \geq 105$ km; = 0 below 105 km

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TABLE II

COMPOSITION AND TOTAL DENSITY AT 120 km, 150 km and 450 km

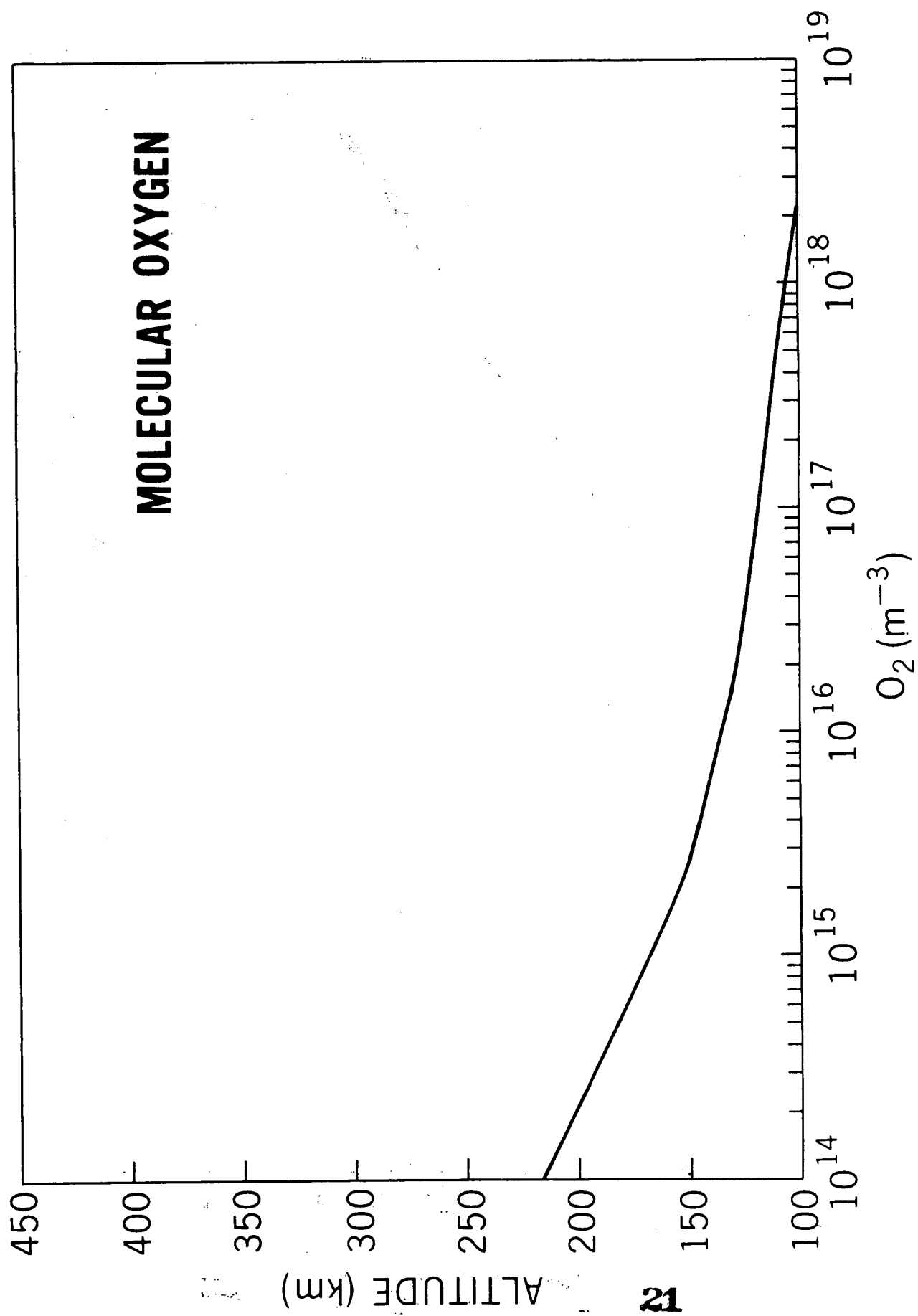|	120 km	150 km	450 km	
N_2	3.71×10^{17}	3.12×10^{16}	1.26×10^{12}	m^{-3}
O	1.01×10^{17}	1.90×10^{16}	4.89×10^{13}	m^{-3}
O_2	6.05×10^{16}	2.75×10^{15}	2.79×10^{10}	m^{-3}
He	2.81×10^{13}	1.50×10^{13}	2.91×10^{12}	m^{-3}
Ar	1.36×10^{15}	5.00×10^{13}	3.24×10^{7}	m^{-3}
ρ	2.33×10^{-8}	2.11×10^{-9}	1.38×10^{-12}	$kg \cdot m^{-3}$
$\overline{M}$	26.22	23.92	15.64	a.m.u.

ALTITUDE (km)

TEMPERATURE

TEMPERATURE

17

TEMPERATURE

ALTITUDE (km)

TEMPERATURE °K

18

MOLECULAR NITROGEN

ALTITUDE (km)

N_2 (m^{-3})

19

MOLECULAR OXYGEN

ALTITUDE (km)

$O_2 (m^{-3})$

20

MOLECULAR OXYGEN

ALTITUDE (km)

O_2 (m^{-3})

21

ATOMIC OXYGEN

ALTITUDE (km)

O (m^{-3})

ATOMIC OXYGEN

ALTITUDE (km)

O (m^{-3})

23

HELIUM

ALTITUDE (km)

He (m^{-3})

ARGON

ALTITUDE (km)

$A(m^{-3})$

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TOTAL MASS DENSITY
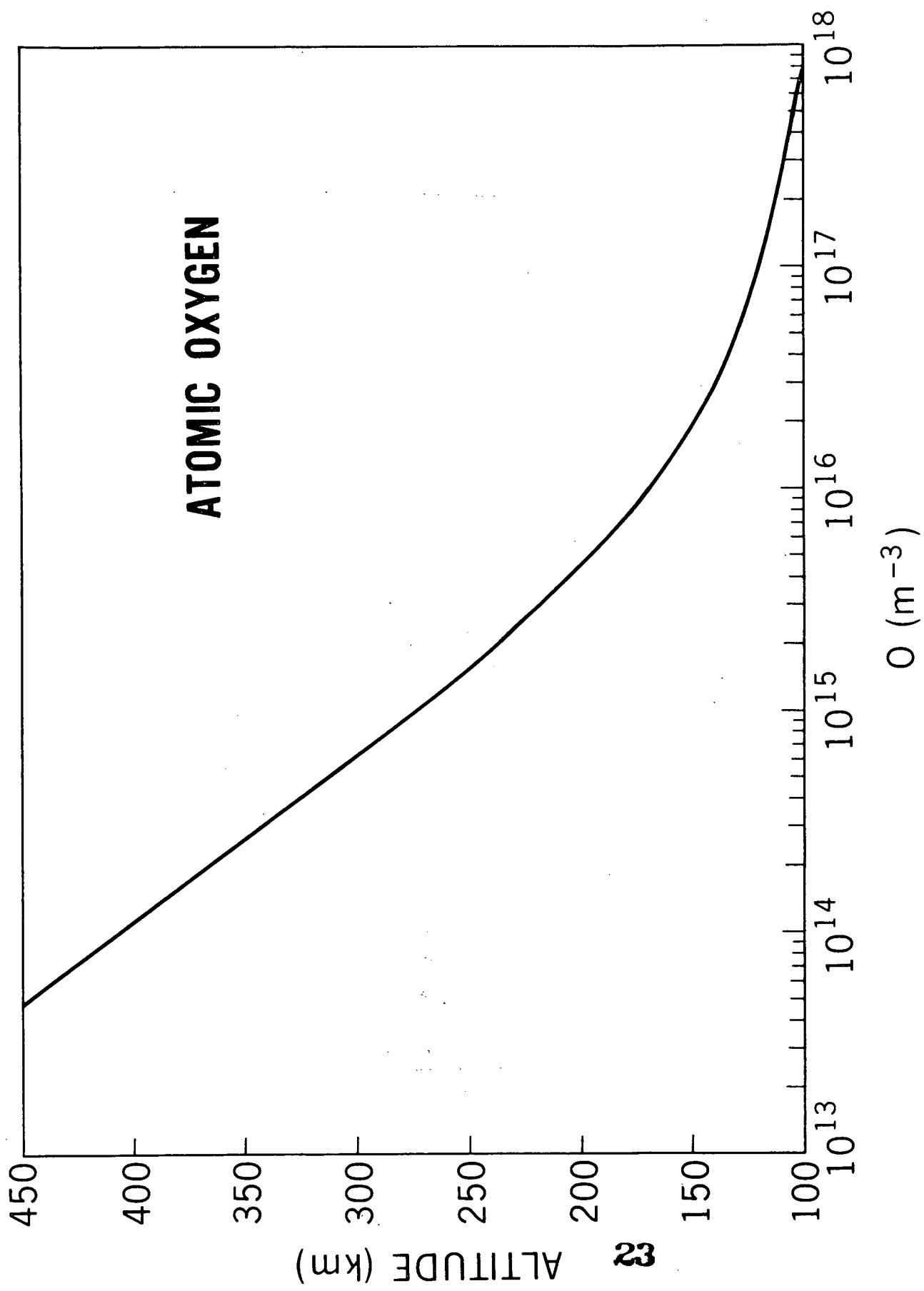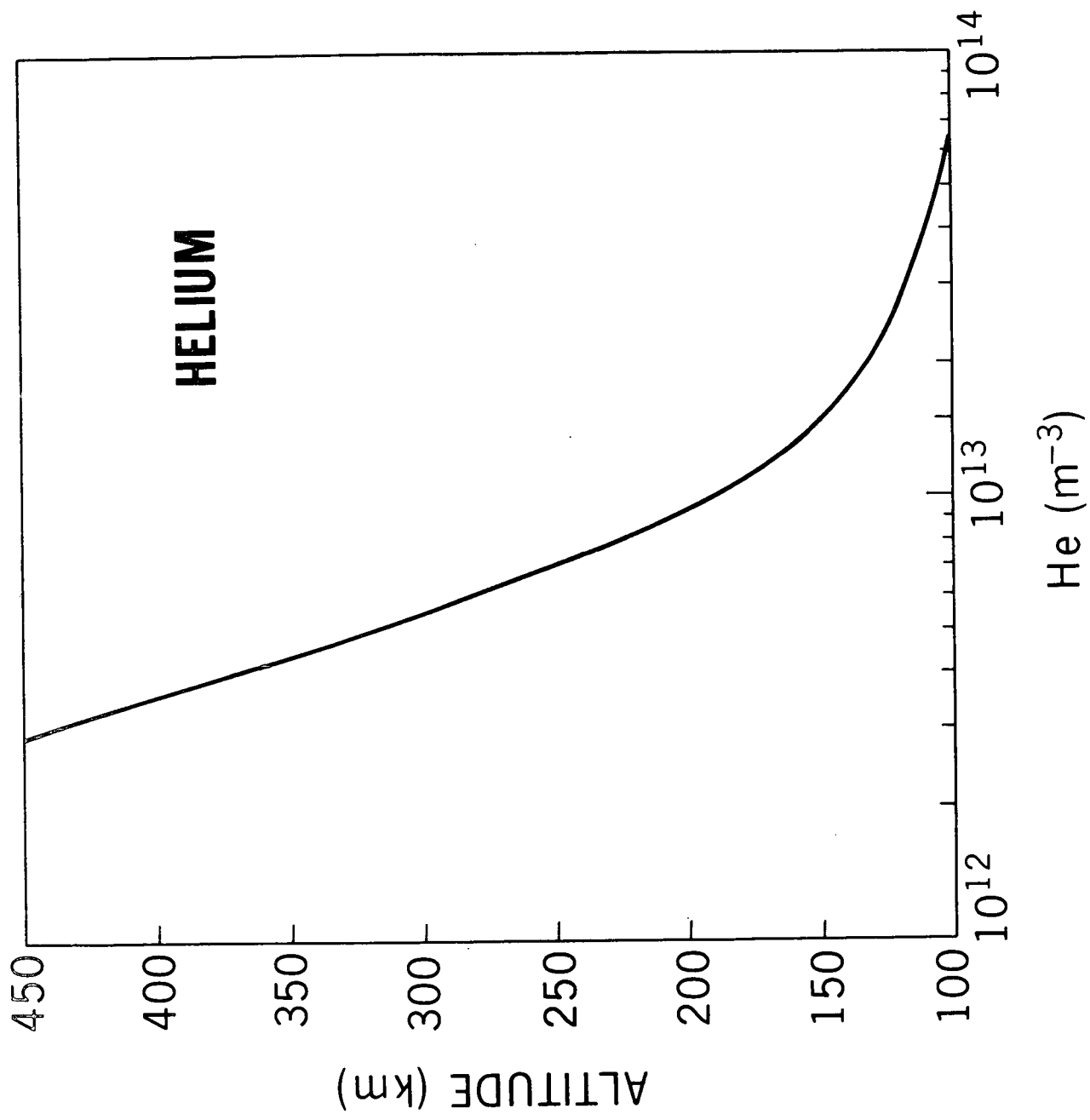
ALTITUDE (km)
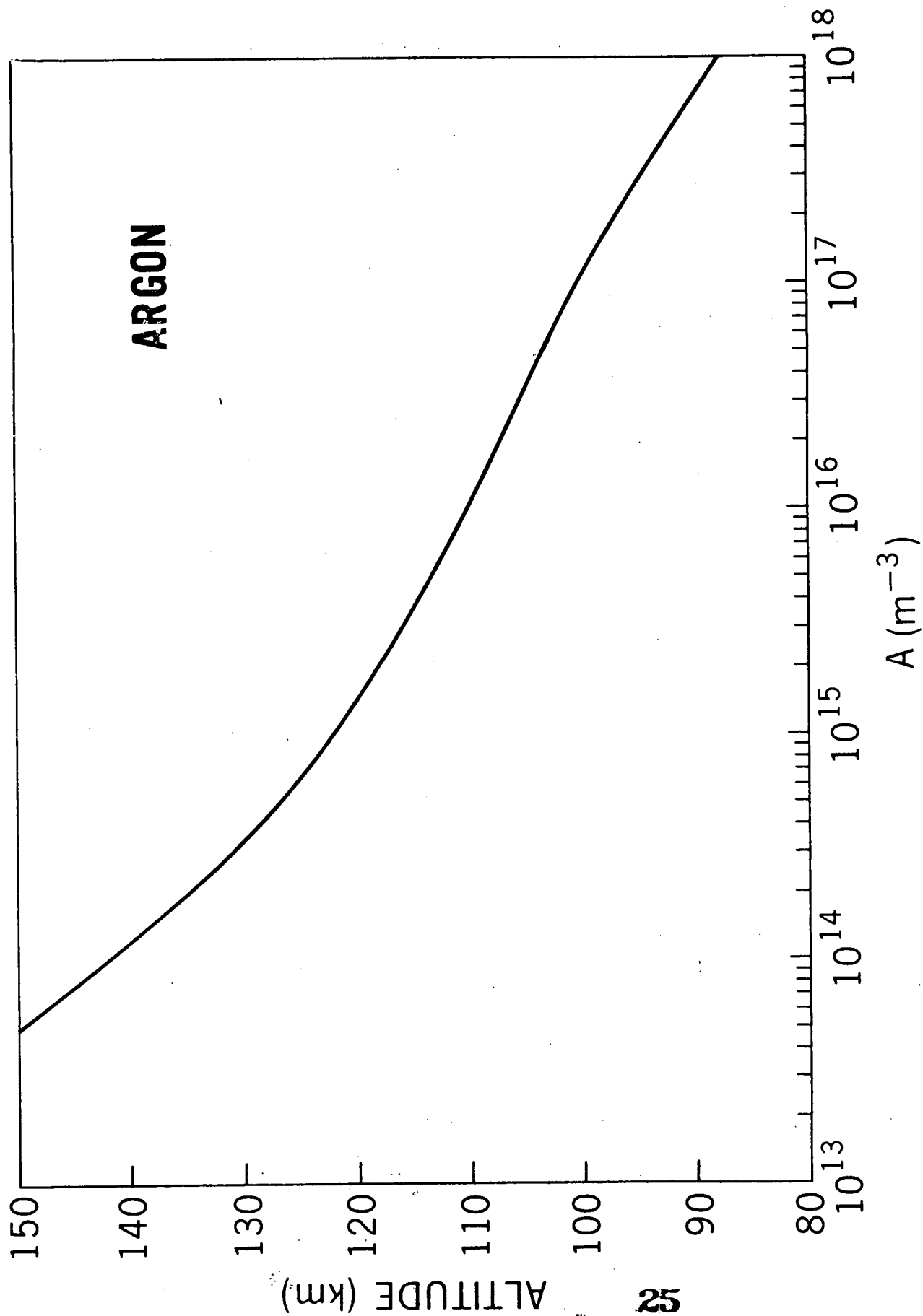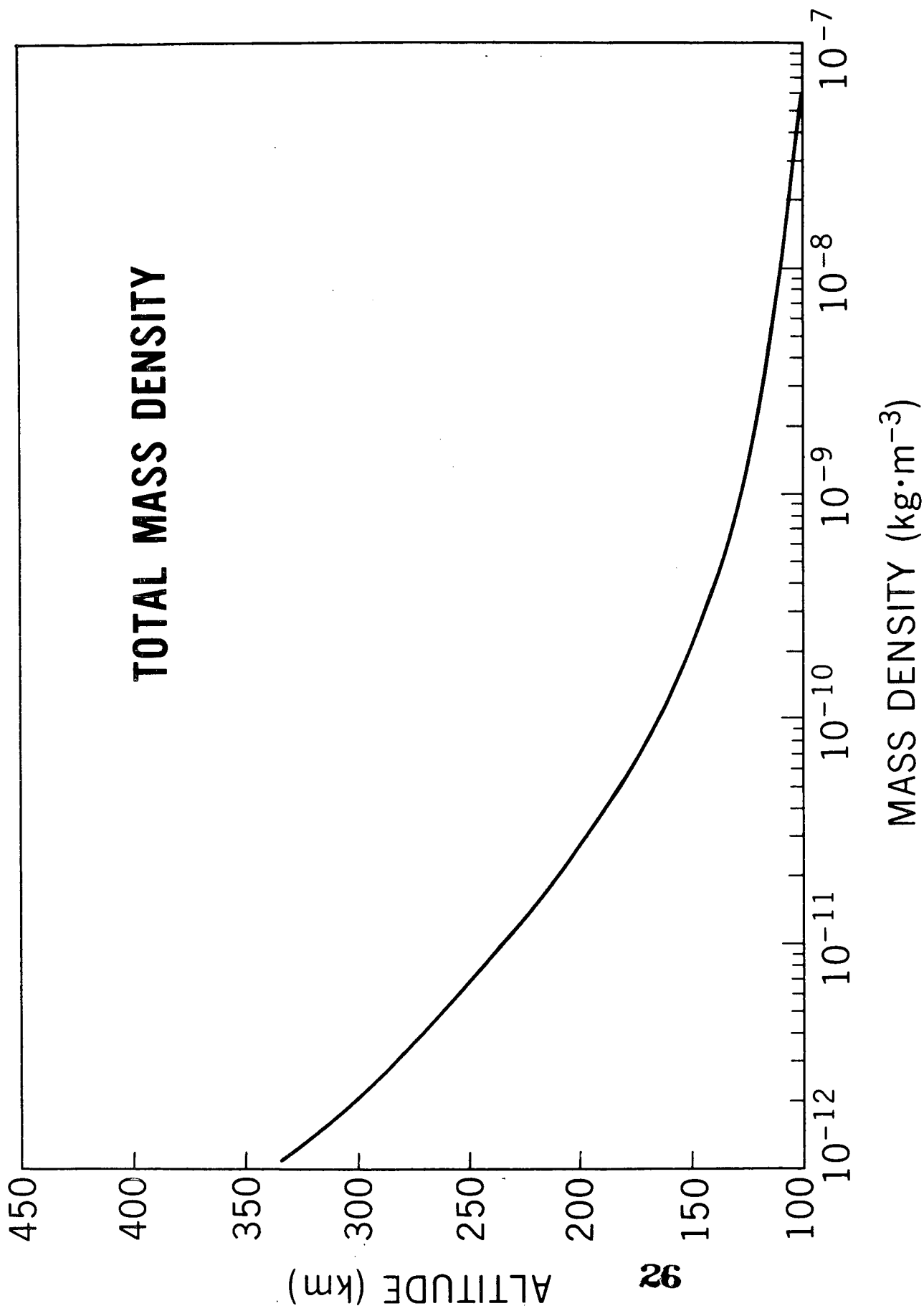
MASS DENSITY (kg·m^{-3})

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includes the provision to represent deviations from diffusive equilibrium profiles in the middle thermosphere which are becoming more and more accepted as physically real.

V. COMPOSITION

Atmospheric densities in the 100-200 km altitude range, computed from composition measurements made with rocket-borne mass spectrometers, have always been lower than values inferred by downward extrapolation of drag measurements on satellites having higher altitude orbits. While it has been recognized that there might be some error in the drag coefficient upon which the drag measurements depended, the general feeling has been that the composition measurements were in error. In particular, because of the highly reactive nature of atomic oxygen it has been assumed that this constituent was largely lost in mass spectrometer ion sources and hence grossly underestimated. Early mass spectrometric values such as those of Meadows and Townsend [1960] or Pokunkov [1960] were extremely low, undoubtedly owing to the loss of atomic oxygen on the extensive surfaces of their instruments. With the advent of "open" source instruments such as those of Schaefer [1963] and of Nier et al. [1964] much higher values were obtained. Even so, it was recognized that the losses might still be considerable.

Hall et al [1965, 1967], using EUV extinction measurements made with rocket-borne UV spectrometers, found atomic oxygen abundances in the 150-200 km altitude range to be considerably above those reported from rocket-borne mass spectrometer measurements. Results extrapolated downward from OSO-III measurements [Hinteregger and Hall, 1969] gave

similar results. The absolute numbers given are in some doubt, however, in view of the uncertainty in the absorption cross section employed for atomic oxygen [Moe, 1970].

vonZahn [1970] summarized the situation at 150 km as of 1970 making use of the relevant published composition values, mass spectroscopic as well as UV extinctions, available at the time. After evaluating the data he concluded that the most consistent agreement between drag and mass spectroscopically determined mass densities was obtained if one assumed that drag determined densities were high by 10% and mass spectroscopically found atomic oxygen values were low by an appreciable factor, perhaps as much as 4. Accordingly he recommended particle densities at 150 km as follows:

$$n(N_2) = 2.6 \times 10^{10} \text{ cm}^{-3}$$
$$n(O_2) = 2.5 \times 10^{9} \text{ cm}^{-3}$$
$$n(Ar) = 5 \times 10^{7}$$
$$n(O) = 2.3 \times 10^{10}$$

and mass density $p = 1.96 \times 10^{-12} \text{ g cm}^{-3}$. His drastic increase in the amount of O seemed justified in part by measurements made at 120 km with a helium-cooled rocket-borne mass spectrometer which gave an appreciably higher value of O/O_2 at 120 km than had ever been reported in the literature [Offermann and von Zahn, 1971].

Nier [1972], on the other hand, pointed out that since atomic oxygen is a major constituent of the atmosphere in the neighborhood of 150 km any arbitrary increase, such as by a factor of substantially more than two in its measured abundance relative to other constituents, would

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destroy the excellent agreement between mass density scale heights computed from mass spectrometer composition measurements and those found from drag measurements on low altitude satellites such as OV1-15 [Champion et al, 1970a] and OV1-16 [Champion et al, 1970b]. He subsequently reinforced his argument through laboratory experiments [Nier et al, 1972] and [Lake and Nier, 1973] in which it was shown that it was not likely that atomic oxygen densities measured with instruments such as he and colleagues previously used in rocket flights were low by a factor of more than two.

More recently Taeusch and Carignan [197] in an extrapolation of OGO-6 composition and drag-determined densities down to 150 km concluded that the 150 km atomic oxygen value given by von Zahn [1970] and employed by Jacchia in his 1971 model was too high. They prefer a number about 20 percent lower but still considerably above the average value found with rocket-borne mass spectrometers. Their $n(N_2)$ and $n(O_2)$ values at 150 km, on the other hand, are about 25 percent higher than values generally found with rocket-borne mass spectrometers.

Moe [1973] completed a comprehensive study of drag measurements with satellites as well as of published values of atmospheric composition by all methods, correcting drag measurements for effects due to accommodation coefficients, and composition measurements for possible errors in instruments due to surface effects. His $n(N_2)$, $n(O_2)$ and $n(Ar)$ values at 150 km agree closely with those given by von Zahn [1970], which are essentially the abundances found by rocket-borne mass spectrometers. His $n(O)$, however, is about 20 percent lower than von Zahn's, in agreement with Taeusch and Carignan [1972].

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The concentration of helium in the lower thermosphere at mid-latitudes is known to vary by a factor of as much as 10 between summer and winter. Also below 150 km it appears not to be in diffusive equilibrium. The values presented in the present report fall between the extremes observed in observations.

While some of the variations reported in $n(N_2)$, $n(O_2)$ and $n(Ar)$ measurements in the 100-200 km range are almost certainly due to errors in measurements, some must be attributed to true atmospheric variations. The values of $n(N_2)$, $n(O_2)$, $n(Ar)$ at 150 km used in constructing the present model are nominal values and are the best estimates at the present time. Each is believed to be correct to 25 percent. Because of the uncertainty in the amount of atomic oxygen lost in rocket-borne mass spectrometers, the value of $n(O)$ at 150 km is based in part on values extrapolated downward from measurements made at higher altitudes with satellite-borne instruments in which it is believed that the atomic oxygen loss can be properly evaluated [Hedin et al, 1973] and in part on mass densities found from satellite drag and corrected for the other constituents (N_2, O_2 and Ar), which can be measured accurately. It appears likely that the $n(O)$ values given in the table are maximum values, as they are based on the assumption that atomic oxygen is strongly absorbed in mass spectrometers used in rocket studies of the lower thermosphere. This view may be too pessimistic but it does not seem probable that values given could be high by a factor as large as two.

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MOLECULAR SCALE TEMPERATURE AND GEOPOTENTIAL

The concept of a "derived 'Temperature' based upon an assumed constant mean molecular weight μ of 28.966 g/mole for the atmosphere" was first applied to atmospheric models in a paper by the Rocket Panel (1952).

The lack of a specific name for this derived "temperature led to the adoption of the name molecular scale temperature in the ARDC Model Atmosphere, 1956 (Minzner, 1956). This concept was carried into the U.S. Extension to the ICAO Standard Atmosphere (Minzner et al., 1958), and into the U.S. Standard Atmosphere, 1962.

The concept of geopotential as a measure of height stems from V. Bjerknes et al., (1910), who "made use of the term 'dynamic height' in referring to the geopotential of a point because the latter is preferable to geometric height in meteorology as a representation of the vertical coordinate of the point" and who "proposed as the unit of geopotential the so-called geodynamic meter (gdm.) or dynamic meter for short" (list, R. J., 1951). With a slight revision in definition, this concept led to the geopotential meter (List, R. J., 1951) and to the standard geopotential meter, the latter of which was first applied explicitly to standard atmospheres in NACA Report 1235, (Annon., 1955). The use of this concept was continued in the ARDC Model Atmosphere, 1956 (Minzner, 1956), in the U. S. Extension to the ICAO Standard Atmosphere (Minzner, et al., 1958) as well as in the U.S. Standard Atmosphere, 1962. The standard

geopotential meter is that unit of geopotential defined in terms of the <u>standard</u> seal-level value of the acceleration of gravity, 9.80665 m sec^{-2}. Implicitly, geopotential has been used as a measure of height in all earlier U.S. Standard Atmospheres in which the tabulated values of pressure were calculated on the basis of a value of the acceleration of gravity, which is invariant with height.

The concept of geopotential has some very meaningful uses in meteorology. In Standard Atmospheres, however, the use of this concept was introduced, either implicitly or explicitly, prior to the development of high-speed digital computers, as a means of avoiding the more complicated equations which result when the pressure-height relationship is developed in terms of an acceleration of gravity varying as some function of height. The use of geopotential has been maintained in all standard atmospheres to date in order to avoid any revision of the lower portion of the tables which have represented the established standard for the past 20 to 50 years.

The introduction of the concept of molecular scale temperature T_M came at a time when standard-atmosphere tables were being extended to heights where the composition, and hence the mean molecular weight were unknown. The use of T_M not only avoided the problem of determining or guessing at a value of mean molecular weight at high altitudes, but also eased the problem of hand or desk-computer calculations by leading to simpler equations than would have resulted if specific height functions had been introduced for both kinetic temperature and mean molecular weight.

In an attempt to further simplify the calculation of standard atmospheres before the wide use of these high-speed computers, Brombacker (1953) attempted to combine the height-dependent acceleration of gravity the height-dependent varying molecular weight and the height-dependent kinetic temperature into a single variable which he called scale-height temperature. This concept, however, was never adopted in standard atmospheres.

In each of the following; the ARDC Model Atmosphere, 1956; the U.S. Extension to the I.C.A.O. Standard Atmosphere; and the ARDC Model Atmosphere 1959 (Minzner, 1959); the entire model was defined in terms of molecular-scale temperature T_M in units of Kelvin degrees K, and geopotential H in units of km . Since most aeronemists were unfamiliar with these quantities and preferred kinetic temperature T, and geometric heights Z it was decided that in the U.S. Standard Atmosphere 1962, the model was divided at 90 geometric kilometers with that part from 0 to 90 km defined in terms of T_M and H, and the part above 90 km defined in terms of T and Z.

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APPENDIX II

COMPLETE TIME DEPENDENT CALCULATION

The philosophy of these calculations is the generation of self consistent

Nitrogen, Oxygen, Ozone and Argon diurnally averaged atmospheres that fall

within the species concentration constraints and altitudes recommended by

Task Group II. The species profiles are the result of a time dependent

photochemical calculation using molecular and turbulent transport which

incorporates the latest measured chemical reaction rates, temperature,

solar flux and turbulent diffusion coefficients into the coupled equations of

motion and continuity.

The species considered are O_1, O_2, O_3, O^1D, $O_2{}^1\Delta_g$, OH, H, HO_2,

H_2O, H_2O_2, H_2 and Ar. The diurnally varying number densities, from 50

to 150 km, are obtained through a finite difference solution of a system of

mass and momentum conservation equations (Shimazaki, 1967; Keneshea and Zim-

merman, 1970). The numerical approach is essentially that introduced

by Shimazaki but modified at the boundaries and in the volume integrations,

following George et al (1972). The chemical production and loss rates for

each species are displayed in the reaction scheme of table 1. The intensity

of the solar flux is that reported in Ackerman (1970)(figure 1) and the

absorption cross sections are those of Hudson (1972). The temperature

profile and the mean molecular mass used up to the turbopause are those

recommended by Task Group II. Using these data, the initial species

distributions are calculated assuming mixing to the turbopause and

diffusive equilibrium above. **38**

The total number density is obtained by integrating the hydrostatic equation where the sea level mass density and the mean molecular weight profiles are taken from the U.S. Standard Atmosphere (1962).

Beginning with the static profiles described above, a steady state solution is determined, which in effect significantly reduces computer time to the final output. The solutions are then continued for ~ 10 days using a fully implicit finite difference technique, a variable time step, limited by species changes of 2 efold and a height step of 100 m. This stringent height step was shown to be necessary to restrict the errors generated by species gradients when height steps larger than 100 m were used.

The turbulent diffusion coefficients used are based upon observations of turbulence in chemical trails, the observed altitudes of cessation and the measured turbulent diffusion coefficients (Zimmerman et al, 1970; Keneshea and Zimmerman, 1970). The turbopause selected was strongly influenced by mass spectrometer measurements (Van Zahn, 1970) where, in general, the reported altitude of transition from mixing to diffusive equilibrium was ~ 102 km. Thus the description of the turbulent diffusion coefficients is given by

$$K = A_1 \exp\left(-2.303 \, \frac{(Z - Z_0)}{a}\right)^2$$

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where the values selected are

$$Z_o = 88 \text{ km},$$

$$a = \begin{cases} 88 \text{ km}, & Z \geq 88 \\ 25 \text{ km}, & Z \leq 88 \end{cases}$$

and

$$A = 3 \times 10^7.$$

The lowest altitude ($\sim$ 50 km) value determined by the above relation approximately matches the reported measurement ($K = 10^5 \text{ cm}^2/\text{sec}$) by Beaudoin et al (1967). The peak value used falls within the experimentally determined values of the vertical turbulent diffusion coefficients (Philbrick et al., 1973), (Keneshea and Zimmerman, 1970). Because of the lack of chemical tracer wind and turbulence measurements in the altitude region 60 to 90 km, we are forced to assume an exponential fit between the measurements at 50 km and 90 km.

RESULTS

The time dependent calculations are continued for $\sim$ 10 days until the species concentrations reproduce themselves within 1% over a diurnal cycle, or what is phrased as arriving at diurnal reproducability. The diurnal average of $[O]$, $[O_2]$, $[O_3]$ and $[Ar]$ is then calculated and extrapolated to 250 km by assuming diffusive equilibrium above the upper boundary. Figures 1 and 2 show the initial conditions of $[N_2]$, Temperature, and the eddy diffusion coefficient used in these one dimensional calculations. Figure 3 shows the diurnally averaged species

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profiles [O], [O$_2$], [O$_3$], [H] and [Ar], with the recommended values of Task Group II at 150 km, also shown. For the turbopause value of ~ 102 km (defined here as the altitude at which the molecular self diffusion coefficient is equal to the turbulent diffusion coefficient) the theoretical values show quite good agreement with the above recommended values at 150 km. Figure 4 presents the argon to nitrogen and the O to O$_2$ ratios. Observe the gradual separation of argon from the mixed region below the turbopause to completely diffusive separation some distance above the turbopause. Because of this fairly large transition region, a simple extrapolation downward of an argon measurement until the ground layer mixing ratio is achieved, can be misleading when trying to describe the turbopause height. This effect, while not shown here, is even greater for helium.

Thus in conclusion, it has been demonstrated that an internally self consistent picture of the density structure of the upper mesosphere and lower thermosphere may be achieved using measured values of solar flux, reaction rates and/or derivatives of measured vertical turbulent transport parameters deduced from chemical trail studies. The fairly good agreement with the limits of these species at 150 km placed upon them by Task Group II may be fortuitous, particularly in the light of the gross differences and uncertainties in the oxygen mass spectrometer measurements. However, it does show that even with

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these uncertainties the physical insight and intuition of Task Group II,
in estimating the above quantities is exceedingly good.

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